Symmetry-breaking bifurcation on the propagation of premixed flames in narrow adiabatic channels for a simple chain-branching kinetics

Daniel Fernández-Galisteo, Carmen Jiménez, and Vadim N. Kurdyumov
Department of Energy, CIEMAT.
Avda. Complutense 40, 28040 Madrid, Spain

1 Introduction

The aim of the present work is to investigate the role of a chain-branching kinetics model in the stability of premixed flames in narrow adiabatic channels and therefore extend the results of previous investigations which made use of a one-step kinetics model [1]. In particular, the work is focused on cases with fuel Lewis number smaller than unity, where symmetry-breaking bifurcation occurs and steady-state flames are stable. The one-step Arrhenius-type model $F + O \rightarrow P$ for the chemistry modeling has been extensively used to better clarify the role of the complex physical phenomena involved in the theoretical studies of flame dynamics in channels [1–5]. Among the most important physical phenomena we distinguish the flame-fluid interaction, the flame-wall interaction and the differential diffusion effect in the flame. The thermo-diffusive approximation, also called constant-density approximation, is used to eliminate the flame-fluid interaction and concentrate on the diffusion effect of the species, either for adiabatic boundary conditions [1, 2, 4] or for the flame-wall heat exchange effects [2, 4, 5] . Before studying the intricate influence of all intermediate or radical species in the flame propagation in small channels by using a detailed chemistry, we propose a theoretical study of the intermediate species effect employing the simpler two-step kinetics model and the thermo-diffusive aproximation.

2 Formulation

Consider a premixed flame propagating in a planar channel at initial tempxerature T_0 and immersed in a Poiseuille flow with mean velocity U_0. In what follows, h denotes the height of the channel and x', y' denote the longitudinal and wall-normal coordinates, respectively. The resulting curved flame separates the frozen mixture, far to the left, from the combustion products downstream to the right. Because this work deals with a diffusive-thermal model, the density of the mixture ρ, the heat capacity c_p, the thermal diffusivity $\mathcal{D}_T$, and the molecular diffusivity of the fuel $\mathcal{D}_F$ and radical $\mathcal{D}_Z$ are all assumed to be constant. As a consecuence, the flow field is not affected by combustion and the flow velocity is given by the Hagen-Poiseuille base flow, $u_{x'} = 6U_0(1 - y'/h)(y'/h)$, and $u_{y'} = 0$.

Correspondence to: d.galisteo@ciemat.es

The mixture is assumed to be deficient in fuel and therefore the mass fraction of the oxidant remains nearly constant. The chemical reaction is modelled by a convenient and simple chain-branching kinetics proposed by Dold [7]. This two-step model includes the branching and recombination steps

$$\begin{aligned} F + Z \rightarrow 2Z \qquad &: \qquad \omega_B = A_B \frac{\rho Y_F}{W_F}\frac{\rho Y_Z}{W_Z}\,\exp\{-E/R^oT\}, \\ Z + M \rightarrow P + M + Q \qquad &: \qquad \omega_C = A_C \frac{\rho Y_Z}{W_Z}\frac{\rho}{W}, \end{aligned} \tag{1}$$

where ω_B is the chain-branching reaction rate, which is thermally sensitive with an activation energy E, and ω_C is the chain-termination reaction rate, independent of the temperature. In what follows, A_B and A_C are the reaction-rate constants, T is the temperature, Y_F and Y_Z are the mass fractions of fuel and radical, M stands for any third body, R^o is the universal gas constant, and W_F, W_Z and W are the fuel, radical and mean molecular weight, respectively. All the heat Q is assumed to be released only in the completion step, being Q the heat released per unit of mole of fuel.

The main feature of this chain-branching chemistry is that it provides the existence of a so-called branching temperature T_c, below which the ratio of removal of radicals by diffusion and recombination exceeds the branching rate. As a consecuence the net branching of radicals is frozen below T_c in the flame. This branching temperature is usually defined by the relation $\omega_B = \beta^2\omega_C$, see [7] for details. The former expression, evaluated at the initial fuel mass fraction Y_{F_0}, being $\beta = E(T_c - T_0)/R^oT_c^2$ the relevant Zel'dovich number based on T_c, reads

$$\frac{A_B}{A_C}\frac{W}{W_F}Y_{F_0} = \left(\frac{E}{R^o}\cdot\frac{T_c - T_0}{T_c^2}\right)^2 \exp\left\{\frac{E}{R^oT_c}\right\}. \tag{2}$$

As done before in [1,4], a reference frame attached to the flame at a point (x'_*, y'_*) is used to develop the formulation. Consider a line paralell to the wall located at a distance $y' = y'_*$. Following the temperature distribution along this line, starting from the unburned side, we choose the first point $x' = x'_*$ where the temperature is equal to some reference value $T = T_*$. The velocity $U_f(t')$ of this point relative to the wall characterizes the time-dependent development of the combustion process.

To clarify the problem, the burning velocity of the planar flame S_L together with the thermal flame thickness, defined as $\delta_T = \mathcal{D}_T/S_L$, are used below to specify the dimensionless parameters. A non-dimensional temperature defined as $\theta = (T - T_0)/(T_c - T_0)$ is also introduced. Choosing h and $h^2/\mathcal{D}_T$ as the reference length and time scales, the non-dimensional coordinates and time become respectively $(x, y) = (x'/h, y'/h)$ and $t = t'/(h^2/\mathcal{D}_T)$, and fuel and radical mass fraction are scaled with the initial mass fraction Y_{F_0} according to $F = Y_F/Y_{F_0}$ and $Z = Y_ZW_F/(Y_{F_0}W_Z)$. Introducing these variables and making use of (2) reduces the conservation equations to the dimensionless form

$$\frac{\partial\theta}{\partial t} + \sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial\theta}{\partial x} = \Delta\theta + d\,\mu qZ \tag{3}$$

$$\frac{\partial F}{\partial t} + \sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial F}{\partial x} = \frac{1}{Le_F}\Delta F - d\,\mu k(\theta)FZ \tag{4}$$

$$\frac{\partial Z}{\partial t} + \sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial Z}{\partial x} = \frac{1}{Le_Z}\Delta Z + d\,\mu k(\theta)FZ - d\,\mu Z, \tag{5}$$

where

$$k(\theta) = \beta^2\exp\left\{\frac{\beta(\theta-1)}{1+\gamma(\theta-1)}\right\}. \tag{6}$$

Herein $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ for a planar channel. The values of the dimensionless burning velocity $u_f(t) = U(t')/S_L$ are calculated by the additional condition $\theta(x_*, y_*; t) = \theta_*$, being $\theta_* = (T_* - T_0)/(T_c - T_0)$ the dimensionless reference temperature at the reference point (x_*, y_*). Eqs. (3)-(6) need to be supplemented by the following boundary conditions far upstream and downstrean of the flame front

$$\begin{aligned} x \to -\infty: &\quad \theta = F - 1 = Z = 0 \\ x \to +\infty: &\quad \partial\theta/\partial x = \partial F/\partial x = \partial Z/\partial x = 0, \end{aligned} \tag{7}$$

and by the boundary conditions at the wall

$$y = 0 \quad \text{and} \quad y = 1: \quad \partial\theta/\partial y = \partial F/\partial y = \partial Z/\partial y = 0, \tag{8}$$

The following non-dimensional parameters appear in the above formulation: the fuel and radical Lewis number Le_F and Le_Z respectively, the heat release parameter $\gamma = (T_c - T_0)/T_c$, the heat of reaction $q = QY_{F_0}/[c_p(T_c - T_0)W_F]$, the flow rate $m = U_0/S_L$, and the reduced Damköhler number as a quotient of diffusion to chemical time $d = h^2 S_L^2/\mathcal{D}_T^2$. The Damköhler number can also be expressed as $d = (h/\delta_T)^2$, the square of the ratio of the channel height to the thermal flame thickness defined above. The parameter $\mu = (\rho A_c \mathcal{D}_T)/(W S_L^2)$ represents the inverse square of the planar flame burning velocity and corresponds with the solution of the one-dimensional eigenvalue problem. This problem and the values of μ were calculated numerically in [8], where the existence of fuel leakage and also multiple solutions for flames with $Le_F > 1$ was demonstrated near the flammability limit when using the chain-branching kinetics model used here. In what follows, the Zel'dovich number and the heat release parameter were kept fixed at $\beta = 5$ and $\gamma = 0.7$, respectively, for all calculations.

3 Symmetry-breaking bifurcation

Both symmetric and non-symmetric steady flame solution were obtained for a constant Damköhler number $d = 20$ and for values of the heat of reaction $q = 2$ and 1.2, the latter corresponding to flames close to the flammability limit. Here, the heat of reaction plays the role of the equivalence ratio for sufficiently lean mixtures, so by using this simple chain-branching model, the influence of the equivalence ratio on the stability of the steady-state flames can be addressed. The propagation velocity of the symmetric flame solution was calculated by reducing the domain to half its height, $0 \le y \le 1/2$, and imposing symmetric boundary conditions for the temperature and species mass fraction, $\partial\theta/\partial y = \partial F/\partial y = \partial Z/\partial y = 0$, in $y = 1/2$. The calculations were carried out in a finite domain, $x_{min} \le x \le x_{max}$, where typical values $x_{min} = -10$ and $x_{max} = 10$ were used in a rectangular grid of 2001×101 points. The independence of the results with the mesh were correspondingly checked. The steady-state calculations were solved using the iterative Gauss-Seidel method with over-relaxation when $\partial/\partial t = 0$ in Eqs. (3)-(5).

Fig. 1 shows the variation of the flame velocity u_f with the dimensionless flow rate m for different fuel Lewis number. Dashed curves indicate unstable symmetric solutions. For sufficiently negative values of m, or assisted flow, the flame is always symmetric. Increasing m to positive values the flame switches to a non-symmetric solution for $Le_F < 1$. When the intermediate specie is very diffusive, case $Le_Z = 0.3$, the symmetric solution can, however, be extended to larger values of m, reducing the critical flash-back point (marked with the symbol $\circ$ in figures) to smaller values of m. The diffusivity of the radicals has a strong effect on the stability of symmetric flames. Radicals diffuse from the highest concentrations located in the more curved part of the flame within the branching zone both to the lowest concentrations in this zone and to the wider recombination zone, promoting then the symmetry in the flame. However, close to the flammability limit, that is for $q = 1.2$, this effect is significantly less pronounced because

of the small radical concentration. The supercritical bifurcation points are marked with •. These points, calculated using the linear stability analysis developed in the next section, are in agreement with the results predicted by the steady-state calculations of symmetric and non-symmetric flames carried out in this section. It is interesting to observe that for mixtures near the flammability limit and at small enough values of Le_F, cellular flames structures may appear, see Fig. 1c). Calculations of the non-symmetric solutions for the cases $q = 1.2$ and $Le_F = 0.3$ where unable to obtain using the numerical techniques specified before.

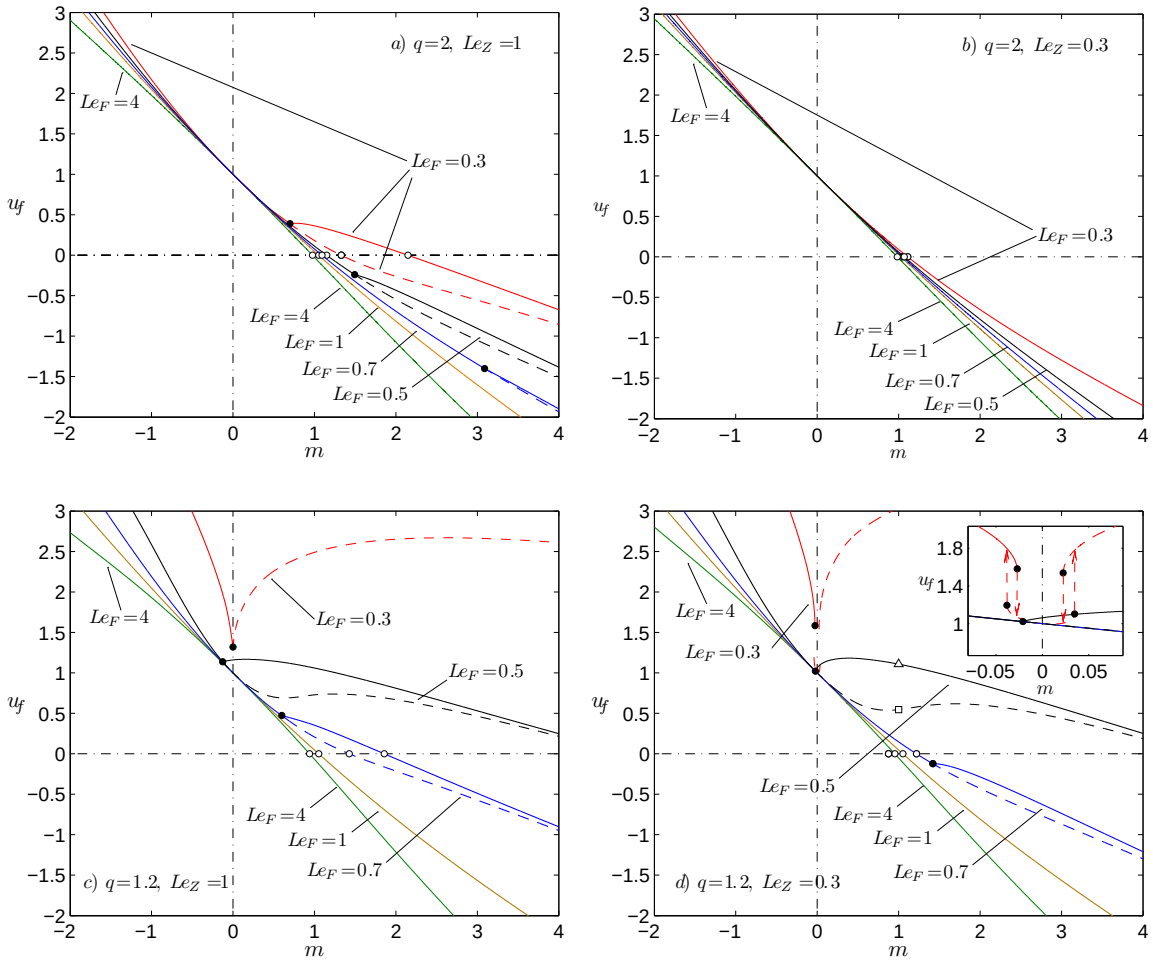

Figure 1: Computed flame velocity $u_f = U_f/S_L$ with the non-dimensional flow rate $m = U_0/S_L$ for different Le_F. For completeness, the corresponding values of μ used in the calculations are specified herein: $a)$ $\mu = 1.3018, 1.0248, 0.8987, 0.7976, 0.5915$; $b)$ $\mu = 1.0737, 0.7924, 0.6759, 0.5891, 0.4349$; $c)$ $\mu = 34.5498, 11.9067, 7.4947, 5.2054, 2.4502$; and $d)$ $\mu = 76.3209, 21.9037, 21.4825, 7.9743, 3.2300$ for $Le_F = 0.3, 0.5, 0.7, 1, 4$, in all cases respectively.

4 Linear stability analysis

The stability analysis of the symmetric steady flames is formulated introducing a small harmonic perturbation in the form: $\theta(x, y; t) = \theta_0(x, y) + \epsilon\, \theta_1(x, y) \exp(\lambda t)$, $F(x, y; t) = F_0(x, y) + \epsilon F_1(x, y) \exp(\lambda t)$,

and $Z(x,y;t) = Z_0(x,y) + \epsilon Z_1(x,y)\exp(\lambda t)$, where $\lambda \in \mathbb{C}$. The subindex 0 denotes the base solution obtained in the steady-state calculations above and ϵ is a small perturbation. As explained in [1], there is no need to introduce a perturbation for u_f in the analysis, so the linearized eigenvalue problem obtained when substituting the perturbation indicated above into Eqs.(3)-(8) leads to the following two-dimensional homogeneous problem

$$\lambda\theta_1 = -\sqrt{d}\{u_f + 6\,my(1-y)\}\frac{\partial\theta_1}{\partial x} + \Delta\theta_1 + d\,\mu q Z_1 \tag{9}$$

$$\lambda F_1 = -\sqrt{d}\{u_f + 6\,my(1-y)\}\frac{\partial F_1}{\partial x} + \frac{1}{Le_F}\Delta F_1 - d\,\mu k(\theta_0)\{A\theta_1 + Z_0F_1 + F_0Z_1\} \tag{10}$$

$$\lambda Z_1 = -\sqrt{d}\{u_f + 6\,my(1-y)\}\frac{\partial Z_1}{\partial x} + \frac{1}{Le_Z}\Delta Z_1 + d\,\mu k(\theta_0)\{A\theta_1 + Z_0F_1 + F_0Z_1\} - d\,\mu Z_1, \tag{11}$$

where $A = \dfrac{\beta}{[1+\gamma(\theta_0-1)]^2}Z_0F_0$. To study the stability of the symmetric steady flames Eqs.(9)-(11) should be considered in half of the domain with the corresponding boundary conditions

$$\begin{aligned} x \to -\infty: &\quad \theta_1 = F_1 = Z_1 = 0 \\ x \to +\infty: &\quad \partial\theta_1/\partial x = \partial F_1/\partial x = \partial Z_1/\partial x = 0, \end{aligned} \tag{12}$$

$$y = 0: \quad \partial\theta_1/\partial y = \partial F_1/\partial y = \partial Z_1/\partial x = 0 \tag{13}$$

and two kinds of boundary conditions in the midplane $y = 1/2$ which select either the symmetric perturbation mode: $\partial\theta_1/\partial y = \partial F_1/\partial y = \partial Z_1/\partial y = 0$ or the non-symmetric perturbation mode: $\theta_1 = F_1 = Z_1 = 0$.

The main goal of the linear stability analysis lies in determine whether a given steady solution is stable or not. Therefore, it is enough to have information about the eigenvalue with the largest real part λ_1, and the present work uses the method developed in [1] for calculating this main eigenvalue. This method is simple to implement with a numerical cost comparable with that needed to calculate an unsteady solution using a time-marching procedure. If the real part of the main eigenvalue obtained is positive, $\mathbb{R}(\lambda_1) > 0$, the steady solution is unstable, and conversely. For the cases studied here, with $Le_F < 1$, only steady solutions emerge and only symmetry-breaking bifurcations where found, so the symmetric mode boundary condition always produces $\lambda_1 = 0$, see [1]. Fig. 3 shows the values of the main eigenvalue for the case $q = 1.2$. The bifurcation points obtained with the stability analysis are marked in Fig. 1 with the symbol •, showing excellent agreement with those found in the steady-state calculations.

5 Conclusion and future work

The present work is focused on the symmetry-breaking bifurcation that appears for $Le_F < 1$ using a simple chain-branching kinetics model. Both symmetric and non-symmetric codes together with a linear stability analysis are employed to investigate steady and stable solutions. We found that the diffusivity of the intermediate species has a strong effect on the stability of symmetric flames, specially away from the flammability limit. It may be interesting to study, in future works, the effect of the intermediate species when pulsating and oscillatory modes appear for $Le_F > 1$ and use the linear stability analysis for predicting those bifurcation points.

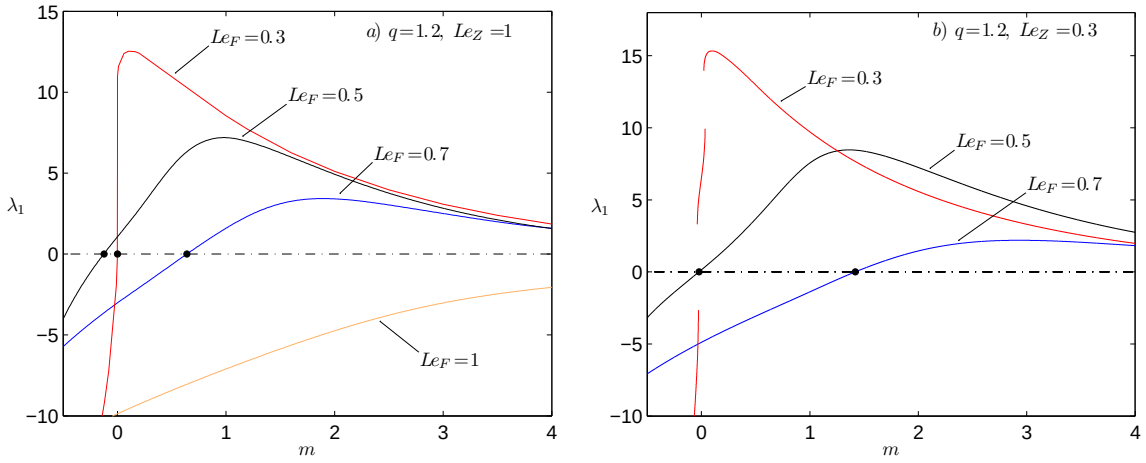

Figure 2: The growth rate of the main eigenvalue λ_1 with the flow rate m for several values of Le_F. Calculated in the case $q = 1.2$: $a)$ $Le_Z = 1$; $b)$ $Le_Z = 0.3$. The case $b)$ for $Le_F = 0.3$ shows four vertical asymptotes due to the double symmetric solution in each branch near $m = 0$, see details in the inset of Fig. $1d)$.

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